PUBCHEM_54605649

40730-78-7 | DTXSID90714109

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.190

Global applicability domain: Inside

Local applicability domain index: 4.36e-01

Confidence level: 6.44e-01

Nearest Neighbors from the Training Set

Image not found

6-Mercaptopurine

Measured: 0.01

Predicted: 1.35e-01